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Supporting Information

Instrumentation and reagents

^{1}H, ^{13}C and ^{19}F NMR spectra were obtained on a Bruker AC250 or a Varian VXR-200 spectrometer. Infrared spectra were measured on a Perkin Elmer 1600 series FT-IR spectrometer. Mass spectra were recorded on a VE Analytical 7070E spectrometer. UV/vis spectra were measured using a Perkin Elmer Lambda 19 spectrophotometer. All solvents used were Aldrich HPLC grade. All chemicals were used as received from Aldrich except for TCNQ and tetrafluoro TCNQ which were obtained from Lancaster Synthesis and Fluorochem respectively.

Crystal, data collection and refinement.

Parameters are given in Table 5. Suitable crystals were selected and mounted on glass fibres with fast-setting epoxy resin. Unit-cell parameters were obtained from 25 reflections (30.90° £ 2q ≤ 37.53°) for compound **3** and 512 reflections (40.60° £ 2q ≤ 7.12°) for compound **6**. Graphite monochromatised Cu Ka radiation was employed for **3** because the crystal diffracted rather weakly. Monochromatic Mo Ka radiation was used for **6**. The structures were solved (Sheldrick, G.M. (1993). SHELX-93. A program for refinement of crystalstructures, University of Göttingen, Germany) using direct methods. Subsequent difference Fourier syntheses were used to locate the remaining atoms. All resulting data were refined by full-matrix least-squares procedures. All data were corrected for Lorentz and polarisation effects. An isotropic extinction correction was applied to the data for **3** [extinction parameter, x = 0.0028(3)] (Extinction parameter = x where F_C is multiplied by $k[1 + 0.001.x.F_C^2 l^3/\sin(2q)]^{-1/4}$ (k = scale factor).). An absorption correction (using integrated φ-scans) was applied to **6**.

In **3**, all non-hydrogen atoms were refined anisotropically and all hydrogen atom thermal parameters were fixed at 120% of the value of their ligated carbon atom.

In **6**, disorder is present (in a ratio of 11:9) in the two terminal ethyl groups such that all non-hydrogen atoms were refined anisotropically except C(19) - C(22). The thermal parameters of these four atoms were fixed at 0.08 $Å^2$. All terminal hydrogen atoms were modelled isotropically at 1.5 v_{iso}(C); all other hydrogen thermal parameters were fixed at 1.2 v_{iso}(C). Dichloromethane solvent was also present in the lattice of **6**, in a molecule : solvent ratio of 1:1. All scattering factors were taken from :- Wilson, A.J.C. (Ed), *International Tables of Crystallography, Vol C, Mathematical, Physical.*, **1992,** Dordrecht, Boston, London. *Tables 4.2.6.8 & 6.1.1.4* . 219-222, 500-503.

X-ray crystallographic data for 3 and 6.

Compound Number (from Figure 2)

	3	6
Molecular formula	$C_{25}H_{28}N_4$	$C_{22}H_{24}N_4O_2.CH_2Cl$
Formula weight	384.51	418.92
Crystal system	Monoclinic	
Space group	$P2_1/n$	C2/c
a (Å)	6.620(1)	44.424(1)
b (Å)	22.050(4)	7.5523(2)
c (Å)	14.845(3)	13.3590(1)
β (°)	99.36(3)	106.386(1)
Volume (Å^3)	2138.1(7)	4299.9(2)
Colour of Crystal	Turquoise	Emerald Green
μ (cm^{-1})	0.553	0.204
Temperature (K)	150	150
Diffractometer type	Rigaku AFC6S	Siemens SMART-CCD
Radiation type	Cu Kα	Mo Kα
θ scan range (°)	3.62 - 74.80	2.74 - 23.23
Reflections collected	4118	7187
Unique reflections	3798	2894
Observed reflections ($I > 2\sigma$)	2143	1409
R1(F) ($I > 2\sigma$)	0.0473	0.0945
wR2(F^2) ($I > 2\sigma$)	0.1114	0.2225
$\Delta / \sigma_{(max)}$	0.001	0.000
$\Delta\rho_{(max, min)}$	0.269 / -0.280	0.369 / -0.398
Data/parameters	3790 / 263	2890 / 250
GOF (on F^2)	1.010	1.090
Z	4	8

Table 1. Crystal data and structure refinement for

Identification code	STRUCTURE 3
Empirical formula	C25 H28 N4
Formula weight	384.51
Temperature	150(2) K
Wavelength	1.54178 A
Crystal system	Monoclinic
Space group	P2(1)/n
Unit cell dimensions	a = 6.620(1) A alpha = 90 deg. b = 22.050(4) A beta = 99.36(3) deg c = 14.845(3) A gamma = 90 deg.
Volume	2138.1(7) A^3
Z	4
Density (calculated)	1.195 Mg/m^3
Absorption coefficient	0.553 mm^-1
F(000)	824
Crystal size	0.55 x 0.125 x 0.075 mm
Theta range for data collection	3.62 to 74.80 deg.
Index ranges	0<=h<=8, 0<=k<=26, -18<=l<=18
Reflections collected	4118
Independent reflections	3798 [R(int) = 0.0350]
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3790 / 0 / 263
Goodness-of-fit on F^2	1.010
Final R indices [I>2sigma(I)]	R1 = 0.0473, wR2 = 0.1114
R indices (all data)	R1 = 0.1276, wR2 = 0.1656
Extinction coefficient	0.0028(3)
Largest diff. peak and hole	0.269 and -0.280 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for dicycnlo[ ]. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
N(1)	14463(4)	5818(1)	4903(2)	37(1)
N(2)	14946(5)	7227(1)	7035(2)	42(1)
N(3)	4723(4)	5825(1)	8835(2)	40(1)
N(4)	2508(4)	4008(1)	7480(2)	23(1)
C(1)	13865(5)	6032(1)	5526(2)	27(1)
C(2)	14121(5)	6806(1)	6689(2)	28(1)
C(3)	13098(5)	6287(1)	6273(2)	25(1)
C(4)	11304(5)	6050(1)	6558(2)	24(1)
C(5)	10282(4)	5530(1)	6130(2)	24(1)
C(6)	8546(5)	5301(1)	6394(2)	25(1)
C(7)	7706(4)	5568(1)	7119(2)	23(1)
C(8)	8705(5)	6089(1)	7537(2)	26(1)
C(9)	10441(5)	6318(1)	7270(2)	26(1)
C(10)	5968(4)	5311(1)	7445(2)	24(1)
C(11)	5317(5)	5608(1)	8224(2)	27(1)
C(12)	4913(4)	4787(1)	7126(2)	23(1)
C(13)	3504(4)	4523(1)	7629(2)	25(1)
C(14)	2658(5)	3621(1)	6669(2)	25(1)
C(15)	559(5)	3412(1)	6186(2)	32(1)
C(16)	817(5)	3033(2)	5349(2)	37(1)
C(17)	2234(5)	2490(2)	5616(2)	37(1)
C(18)	4320(5)	2697(1)	6115(2)	34(1)
C(19)	4090(5)	3082(1)	6950(2)	29(1)
C(20)	1346(5)	3778(1)	8196(2)	24(1)
C(21)	2773(5)	3657(2)	9093(2)	28(1)
C(22)	1544(5)	3423(1)	9811(2)	30(1)
C(23)	-122(5)	3877(2)	9951(2)	34(1)
C(24)	-1563(5)	3987(2)	9057(2)	36(1)
C(25)	-386(5)	4213(2)	8313(2)	31(1)

Table 3. Bond lengths [A] and angles [deg] for dicycnlo, (3)

N(1)-C(1)	1.165(4)
N(2)-C(2)	1.153(4)
N(3)-C(11)	1.149(4)
N(4)-C(13)	1.314(4)
N(4)-C(14)	1.491(4)
N(4)-C(20)	1.497(4)
C(1)-C(3)	1.409(4)
C(2)-C(3)	1.419(4)
C(3)-C(4)	1.423(4)
C(4)-C(9)	1.410(4)
C(4)-C(5)	1.429(4)
C(5)-C(6)	1.369(4)
C(5)-H(5A)	0.96
C(6)-C(7)	1.417(4)
C(6)-H(6A)	0.96
C(7)-C(8)	1.418(4)
C(7)-C(10)	1.435(4)
C(8)-C(9)	1.372(4)
C(8)-H(8A)	0.96
C(9)-H(9A)	0.96
C(10)-C(12)	1.393(4)
C(10)-C(11)	1.454(4)
C(12)-C(13)	1.412(4)
C(12)-H(12A)	0.96
C(13)-H(13A)	0.96
C(14)-C(15)	1.528(4)
C(14)-C(19)	1.536(4)
C(14)-H(14A)	0.96
C(15)-C(16)	1.529(4)
C(15)-H(15A)	0.96
C(15)-H(15B)	0.96
C(16)-C(17)	1.534(5)
C(16)-H(16A)	0.96
C(16)-H(16B)	0.96
C(17)-C(18)	1.527(5)
C(17)-H(17A)	0.96
C(17)-H(17B)	0.96
C(18)-C(19)	1.530(4)
C(18)-H(18A)	0.96
C(18)-H(18B)	0.96
C(19)-H(19A)	0.96
C(19)-H(19B)	0.96
C(20)-C(25)	1.526(4)
C(20)-C(21)	1.526(4)
C(20)-H(20A)	0.96
C(21)-C(22)	1.531(4)
C(21)-H(21A)	0.96
C(21)-H(21B)	0.96
C(22)-C(23)	1.529(4)
C(22)-H(22A)	0.96
C(22)-H(22B)	0.96
C(23)-C(24)	1.523(5)
C(23)-H(23A)	0.96
C(23)-H(23B)	0.96
C(24)-C(25)	1.535(4)
C(24)-H(24A)	0.96
C(24)-H(24B)	0.96
C(25)-H(25A)	0.96
C(25)-H(25B)	0.96

C(13)-N(4)-C(14)	122.2(2)
C(13)-N(4)-C(20)	118.3(2)
C(14)-N(4)-C(20)	119.3(2)
N(1)-C(1)-C(3)	178.8(4)
N(2)-C(2)-C(3)	179.4(3)
C(1)-C(3)-C(2)	117.2(3)
C(1)-C(3)-C(4)	120.8(3)
C(2)-C(3)-C(4)	121.9(3)
C(9)-C(4)-C(3)	121.9(3)
C(9)-C(4)-C(5)	116.7(3)
C(3)-C(4)-C(5)	121.4(3)
C(6)-C(5)-C(4)	121.8(3)
C(6)-C(5)-H(5A)	118.1(2)
C(4)-C(5)-H(5A)	119.8(2)
C(5)-C(6)-C(7)	121.1(3)
C(5)-C(6)-H(6A)	119.9(2)
C(7)-C(6)-H(6A)	118.7(2)
C(6)-C(7)-C(8)	117.2(3)
C(6)-C(7)-C(10)	121.9(3)
C(8)-C(7)-C(10)	120.9(3)
C(9)-C(8)-C(7)	121.7(3)
C(9)-C(8)-H(8A)	118.7(2)
C(7)-C(8)-H(8A)	119.7(2)
C(8)-C(9)-C(4)	121.5(3)
C(8)-C(9)-H(9A)	119.4(2)
C(4)-C(9)-H(9A)	119.1(2)
C(12)-C(10)-C(7)	126.7(3)
C(12)-C(10)-C(11)	116.6(3)
C(7)-C(10)-C(11)	116.6(3)
N(3)-C(11)-C(10)	176.7(3)
C(10)-C(12)-C(13)	120.0(3)
C(10)-C(12)-H(12A)	120.5(2)
C(13)-C(12)-H(12A)	119.5(2)
N(4)-C(13)-C(12)	128.6(3)
N(4)-C(13)-H(13A)	116.8(2)
C(12)-C(13)-H(13A)	114.5(2)
N(4)-C(14)-C(15)	112.1(2)
N(4)-C(14)-C(19)	110.1(2)
C(15)-C(14)-C(19)	111.6(2)
N(4)-C(14)-H(14A)	107.3(1)
C(15)-C(14)-H(14A)	106.4(2)
C(19)-C(14)-H(14A)	109.2(2)
C(14)-C(15)-C(16)	109.5(3)
C(14)-C(15)-H(15A)	109.8(2)
C(16)-C(15)-H(15A)	110.4(2)
C(14)-C(15)-H(15B)	108.9(2)
C(16)-C(15)-H(15B)	109.7(2)
H(15A)-C(15)-H(15B)	108.6
C(15)-C(16)-C(17)	111.2(3)
C(15)-C(16)-H(16A)	108.8(2)
C(17)-C(16)-H(16A)	109.5(2)
C(15)-C(16)-H(16B)	110.1(2)
C(17)-C(16)-H(16B)	109.2(2)
H(16A)-C(16)-H(16B)	108.0
C(18)-C(17)-C(16)	111.0(3)
C(18)-C(17)-H(17A)	110.4(2)
C(16)-C(17)-H(17A)	109.5(2)
C(18)-C(17)-H(17B)	108.4(2)
C(16)-C(17)-H(17B)	109.5(2)
H(17A)-C(17)-H(17B)	108.0
C(17)-C(18)-C(19)	111.0(3)
C(17)-C(18)-H(18A)	108.6(2)
C(19)-C(18)-H(18A)	110.4(2)
C(17)-C(18)-H(18B)	109.7(2)

C(19)-C(18)-H(18B)	108.9(2)
H(18A)-C(18)-H(18B)	108.2
C(18)-C(19)-C(14)	110.3(3)
C(18)-C(19)-H(19A)	109.9(2)
C(14)-C(19)-H(19A)	110.4(2)
C(18)-C(19)-H(19B)	109.1(2)
C(14)-C(19)-H(19B)	109.1(2)
H(19A)-C(19)-H(19B)	107.9
N(4)-C(20)-C(25)	110.5(2)
N(4)-C(20)-C(21)	111.2(2)
C(25)-C(20)-C(21)	112.3(2)
N(4)-C(20)-H(20A)	107.3(1)
C(25)-C(20)-H(20A)	107.9(2)
C(21)-C(20)-H(20A)	107.2(2)
C(20)-C(21)-C(22)	110.1(2)
C(20)-C(21)-H(21A)	110.0(2)
C(22)-C(21)-H(21A)	110.6(2)
C(20)-C(21)-H(21B)	109.1(2)
C(22)-C(21)-H(21B)	109.0(2)
H(21A)-C(21)-H(21B)	108.1
C(23)-C(22)-C(21)	110.6(3)
C(23)-C(22)-H(22A)	107.1(2)
C(21)-C(22)-H(22A)	108.9(2)
C(23)-C(22)-H(22B)	111.5(2)
C(21)-C(22)-H(22B)	110.6(2)
H(22A)-C(22)-H(22B)	108.1
C(24)-C(23)-C(22)	110.4(3)
C(24)-C(23)-H(23A)	109.9(2)
C(22)-C(23)-H(23A)	111.0(2)
C(24)-C(23)-H(23B)	108.5(2)
C(22)-C(23)-H(23B)	109.2(2)
H(23A)-C(23)-H(23B)	107.7
C(23)-C(24)-C(25)	111.1(3)
C(23)-C(24)-H(24A)	108.6(2)
C(25)-C(24)-H(24A)	108.5(2)
C(23)-C(24)-H(24B)	110.4(2)
C(25)-C(24)-H(24B)	110.2(2)
H(24A)-C(24)-H(24B)	108.0
C(20)-C(25)-C(24)	110.9(3)
C(20)-C(25)-H(25A)	108.1(2)
C(24)-C(25)-H(25A)	109.3(2)
C(20)-C(25)-H(25B)	110.4(2)
C(24)-C(25)-H(25B)	110.2(2)
H(25A)-C(25)-H(25B)	108.0

Symmetry transformations used to generate equivalent atoms:

Table 4.Anisotropic displacement parameters (A^2 x 10^3) for dicycnlo,(3)
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
N(1)	40(2)	39(2)	33(2)	-5(1)	8(1)	-11(1)
N(2)	40(2)	31(2)	56(2)	-6(1)	12(2)	-7(1)
N(3)	40(2)	41(2)	40(2)	-13(1)	11(1)	-10(1)
N(4)	24(1)	23(1)	23(1)	0(1)	6(1)	-1(1)
C(1)	26(2)	24(2)	29(2)	3(1)	3(1)	-5(1)
C(2)	26(2)	23(2)	35(2)	1(1)	7(1)	1(1)
C(3)	27(2)	21(2)	25(2)	0(1)	5(1)	1(1)
C(4)	24(2)	21(2)	24(2)	1(1)	1(1)	0(1)
C(5)	23(2)	28(2)	22(1)	0(1)	4(1)	-3(1)
C(6)	30(2)	21(2)	24(1)	0(1)	5(1)	-4(1)
C(7)	24(2)	21(2)	24(1)	1(1)	3(1)	1(1)
C(8)	26(2)	25(2)	26(2)	-3(1)	6(1)	1(1)
C(9)	27(2)	20(2)	31(2)	-4(1)	5(1)	-4(1)
C(10)	24(2)	22(2)	23(1)	1(1)	0(1)	3(1)
C(11)	27(2)	23(2)	30(2)	-3(1)	5(1)	-4(1)
C(12)	22(2)	23(2)	23(1)	2(1)	4(1)	0(1)
C(13)	24(2)	24(2)	27(2)	1(1)	3(1)	1(1)
C(14)	31(2)	22(2)	24(1)	-2(1)	8(1)	-2(1)
C(15)	30(2)	28(2)	34(2)	-2(1)	-1(1)	4(1)
C(16)	45(2)	30(2)	32(2)	-5(1)	-5(2)	1(2)
C(17)	51(2)	25(2)	34(2)	-6(1)	5(2)	3(2)
C(18)	43(2)	26(2)	33(2)	-2(1)	9(2)	4(1)
C(19)	30(2)	28(2)	28(2)	-1(1)	3(1)	2(1)
C(20)	24(2)	24(2)	24(1)	2(1)	6(1)	-5(1)
C(21)	30(2)	29(2)	25(2)	1(1)	5(1)	0(1)
C(22)	34(2)	32(2)	23(2)	4(1)	3(1)	-4(1)
C(23)	38(2)	33(2)	32(2)	-2(1)	10(2)	-5(2)
C(24)	30(2)	42(2)	38(2)	5(2)	11(2)	1(2)
C(25)	28(2)	33(2)	32(2)	9(1)	8(1)	4(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for dicycnlo$_5$(3)

	x	y	z	U(eq)
H(5A)	10731(4)	5355(1)	5604(2)	29
H(6A)	7959(5)	4931(1)	6129(2)	30
H(8A)	8158(5)	6290(1)	8018(2)	31
H(9A)	11081(5)	6670(1)	7572(2)	31
H(12A)	5135(4)	4603(1)	6565(2)	28
H(13A)	3236(4)	4760(1)	8139(2)	30
H(14A)	3224(5)	3868(1)	6239(2)	30
H(15A)	-293(5)	3758(1)	6008(2)	38
H(15B)	-73(5)	3171(1)	6602(2)	38
H(16A)	1385(5)	3286(2)	4926(2)	44
H(16B)	-491(5)	2890(2)	5051(2)	44
H(17A)	2389(5)	2264(2)	5078(2)	44
H(17B)	1631(5)	2226(2)	6014(2)	44
H(18A)	4988(5)	2926(1)	5698(2)	40
H(18B)	5153(5)	2350(1)	6311(2)	40
H(19A)	3573(5)	2837(1)	7396(2)	35
H(19B)	5411(5)	3231(1)	7222(2)	35
H(20A)	745(5)	3397(1)	7984(2)	29
H(21A)	3499(5)	4020(2)	9302(2)	34
H(21B)	3760(5)	3355(2)	8994(2)	34
H(22A)	2444(5)	3385(1)	10384(2)	36
H(22B)	979(5)	3031(1)	9643(2)	36
H(23A)	465(5)	4255(2)	10188(2)	41
H(23B)	-901(5)	3716(2)	10387(2)	41
H(24A)	-2541(5)	4291(2)	9156(2)	43
H(24B)	-2300(5)	3623(2)	8860(2)	43
H(25A)	-1302(5)	4235(2)	7742(2)	37
H(25B)	145(5)	4612(2)	8459(2)	37

Table 1. Crystal data and structure refinement for 6

Identification code	UltraDemi
Empirical formula	C22.50 H25 Cl N4 O2
Formula weight	418.92
Temperature	150(2) K
Wavelength	0.71073 A
Crystal system	monoclinic
Space group	C2/c
Unit cell dimensions	a = 44.424(1) A alpha = 90 deg. b = 7.5523(2) A beta = 106.386(1) deg c = 13.3590(1) A gamma = 90 deg.
Volume	4299.9(2) A^3
Z	8
Density (calculated)	1.294 Mg/m^3
Absorption coefficient	0.204 mm^-1
F(000)	1768
Crystal size	0.32 x 0.28 x 0.03 mm
Theta range for data collection	2.74 to 23.24 deg.
Index ranges	-45<=h<=48, -8<=k<=7, -14<=l<=14
Reflections collected	7187
Independent reflections	2894 [R(int) = 0.1554]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2890 / 0 / 250
Goodness-of-fit on F^2	1.090
Final R indices [I>2sigma(I)]	R1 = 0.0945, wR2 = 0.2225
R indices (all data)	R1 = 0.1902, wR2 = 0.2979
Largest diff. peak and hole	0.369 and -0.398 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for UltraDemi. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1)	571(2)	9101(7)	4129(5)	62(2)
O(2)	691(2)	11770(7)	4955(5)	62(2)
N(1)	3407(2)	18088(8)	7150(6)	57(2)
N(2)	3783(2)	12850(8)	8149(5)	47(2)
N(3)	2084(2)	8325(7)	5651(5)	38(2)
N(4)	1248(2)	11975(6)	4353(5)	34(2)
C(1)	3360(2)	16620(10)	7223(6)	39(2)
C(2)	3564(2)	13688(10)	7771(6)	40(2)
C(3)	3299(2)	14743(8)	7291(6)	33(2)
C(4)	2998(2)	14028(8)	6918(5)	29(2)
C(5)	2731(2)	15085(8)	6478(6)	31(2)
C(6)	2437(2)	14411(8)	6094(6)	34(2)
C(7)	2383(2)	12540(7)	6135(5)	27(2)
C(8)	2649(2)	11478(8)	6557(5)	31(2)
C(9)	2941(2)	12160(8)	6934(6)	34(2)
C(10)	2082(2)	11763(7)	5719(5)	27(2)
C(11)	2084(2)	9844(8)	5694(6)	31(2)
C(12)	1784(2)	12514(7)	5320(6)	29(2)
C(13)	1721(2)	14493(8)	5323(6)	35(2)
C(14)	1376(2)	14866(8)	5138(6)	43(2)
C(15)	1177(1)	13896(6)	4182(4)	39(2)
C(16)	1525(1)	11410(6)	4857(4)	29(2)
C(17)	991(2)	10719(8)	3885(6)	39(2)
C(18)	817(2)	10232(9)	4650(6)	43(2)
C(19A)	597(5)	7435(26)	4485(17)	80
C(19B)	458(7)	7861(31)	4697(19)	80
C(20)	283(3)	6442(13)	4036(8)	74(3)
C(21A)	685(5)	11659(29)	6063(17)	80
C(21B)	555(7)	11740(36)	5772(20)	80
C(22)	675(3)	13266(15)	6503(9)	93(4)
Cl(1)	-240(1)	2618(4)	3052(2)	93(1)
C(23)	0	1337(15)	2500	87(5)

Table 3. Bond lengths [A] and angles [deg] for UltraDemi. (6)

O(1)-C(19A)	1.34(2)
O(1)-C(19B)	1.39(2)
O(1)-C(18)	1.406(9)
O(2)-C(21B)	1.39(3)
O(2)-C(18)	1.399(9)
O(2)-C(21A)	1.49(2)
N(1)-C(1)	1.137(8)
N(2)-C(2)	1.15(1)
N(3)-C(11)	1.149(7)
N(4)-C(16)	1.296(8)
N(4)-C(17)	1.479(9)
N(4)-C(15)	1.489(6)
C(1)-C(3)	1.45(1)
C(2)-C(3)	1.42(1)
C(3)-C(4)	1.40(1)
C(4)-C(5)	1.41(1)
C(4)-C(9)	1.434(9)
C(5)-C(6)	1.36(1)
C(5)-H(5)	0.95
C(6)-C(7)	1.437(9)
C(6)-H(6)	0.95
C(7)-C(8)	1.41(1)
C(7)-C(10)	1.42(1)
C(8)-C(9)	1.36(1)
C(8)-H(8)	0.95
C(9)-H(9)	0.95
C(10)-C(12)	1.40(1)
C(10)-C(11)	1.450(9)
C(12)-C(16)	1.416(9)
C(12)-C(13)	1.521(8)
C(13)-C(14)	1.51(1)
C(13)-H(13A)	0.99
C(13)-H(13B)	0.99
C(14)-C(15)	1.522(9)
C(14)-H(14A)	0.99
C(14)-H(14B)	0.99
C(15)-H(15A)	0.99
C(15)-H(15B)	0.99
C(16)-H(16)	0.95
C(17)-C(18)	1.49(1)
C(17)-H(17A)	0.99
C(17)-H(17B)	0.99
C(18)-H(18)	1.00
C(19A)-C(20)	1.55(2)
C(19A)-H(19A)	0.99
C(19A)-H(19B)	0.99
C(19B)-C(20)	1.47(3)
C(19B)-H(19C)	0.99
C(19B)-H(19D)	0.99
C(20)-H(20A)	0.99(1)
C(20)-H(20B)	0.95(1)
C(20)-H(20C)	0.97(1)
C(20)-H(20D)	0.99(1)
C(20)-H(20E)	0.96(1)
C(20)-H(20F)	0.95(1)
C(21A)-C(22)	1.35(2)
C(21A)-H(21A)	0.99
C(21A)-H(21B)	0.99
C(21B)-C(22)	1.51(3)
C(21B)-H(21C)	0.99

C(21B)-H(21D)	0.99
C(22)-H(22A)	0.94(1)
C(22)-H(22B)	0.95(1)
C(22)-H(22C)	0.99(1)
C(22)-H(22D)	0.95(1)
C(22)-H(22E)	0.99(1)
C(22)-H(22F)	0.94(1)
Cl(1)-C(23)	1.748(7)
C(23)-Cl(1)#1	1.748(7)
C(23)-H(23A)	0.99
C(23)-H(23B)	0.99

C(19A)-O(1)-C(18)	115(1)
C(19B)-O(1)-C(18)	119(1)
C(21B)-O(2)-C(18)	121(1)
C(18)-O(2)-C(21A)	111(1)
C(16)-N(4)-C(17)	120.9(5)
C(16)-N(4)-C(15)	122.1(6)
C(17)-N(4)-C(15)	117.0(6)
N(1)-C(1)-C(3)	179(1)
N(2)-C(2)-C(3)	178.6(9)
C(4)-C(3)-C(2)	122.3(6)
C(4)-C(3)-C(1)	122.1(7)
C(2)-C(3)-C(1)	115.6(7)
C(3)-C(4)-C(5)	122.5(6)
C(3)-C(4)-C(9)	121.9(7)
C(5)-C(4)-C(9)	115.6(7)
C(6)-C(5)-C(4)	123.3(6)
C(6)-C(5)-H(5)	118.3(4)
C(4)-C(5)-H(5)	118.3(4)
C(5)-C(6)-C(7)	120.4(7)
C(5)-C(6)-H(6)	119.8(4)
C(7)-C(6)-H(6)	119.8(5)
C(8)-C(7)-C(10)	120.8(6)
C(8)-C(7)-C(6)	116.5(7)
C(10)-C(7)-C(6)	122.6(7)
C(9)-C(8)-C(7)	122.7(6)
C(9)-C(8)-H(8)	118.7(4)
C(7)-C(8)-H(8)	118.7(4)
C(8)-C(9)-C(4)	121.4(7)
C(8)-C(9)-H(9)	119.3(4)
C(4)-C(9)-H(9)	119.3(5)
C(12)-C(10)-C(7)	131.8(6)
C(12)-C(10)-C(11)	114.0(7)
C(7)-C(10)-C(11)	114.2(7)
N(3)-C(11)-C(10)	178.5(9)
C(10)-C(12)-C(16)	119.6(5)
C(10)-C(12)-C(13)	123.5(7)
C(16)-C(12)-C(13)	116.9(7)
C(14)-C(13)-C(12)	111.2(6)
C(14)-C(13)-H(13A)	109.4(4)
C(12)-C(13)-H(13A)	109.4(4)
C(14)-C(13)-H(13B)	109.4(4)
C(12)-C(13)-H(13B)	109.4(4)
H(13A)-C(13)-H(13B)	108.0
C(13)-C(14)-C(15)	111.9(5)
C(13)-C(14)-H(14A)	109.2(3)
C(15)-C(14)-H(14A)	109.2(3)
C(13)-C(14)-H(14B)	109.2(4)
C(15)-C(14)-H(14B)	109.2(3)
H(14A)-C(14)-H(14B)	107.9
N(4)-C(15)-C(14)	107.0(5)
N(4)-C(15)-H(15A)	110.3(3)
C(14)-C(15)-H(15A)	110.3(4)

N(4)-C(15)-H(15B)	110.3(5)
C(14)-C(15)-H(15B)	110.3(3)
H(15A)-C(15)-H(15B)	108.6
N(4)-C(16)-C(12)	124.7(5)
N(4)-C(16)-H(16)	117.7(3)
C(12)-C(16)-H(16)	117.7(3)
N(4)-C(17)-C(18)	110.9(6)
N(4)-C(17)-H(17A)	109.5(4)
C(18)-C(17)-H(17A)	109.5(4)
N(4)-C(17)-H(17B)	109.5(4)
C(18)-C(17)-H(17B)	109.5(5)
H(17A)-C(17)-H(17B)	108.1
O(2)-C(18)-O(1)	109.3(7)
O(2)-C(18)-C(17)	108.8(6)
O(1)-C(18)-C(17)	107.0(6)
O(2)-C(18)-H(18)	110.6(4)
O(1)-C(18)-H(18)	110.6(4)
C(17)-C(18)-H(18)	110.6(5)
O(1)-C(19A)-C(20)	110(2)
O(1)-C(19A)-H(19A)	109.7(9)
C(20)-C(19A)-H(19A)	109.7(9)
O(1)-C(19A)-H(19B)	110(1)
C(20)-C(19A)-H(19B)	109.7(9)
H(19A)-C(19A)-H(19B)	108.2
O(1)-C(19B)-C(20)	112(2)
O(1)-C(19B)-H(19C)	109(1)
C(20)-C(19B)-H(19C)	109(1)
O(1)-C(19B)-H(19D)	109(1)
C(20)-C(19B)-H(19D)	109(1)
H(19C)-C(19B)-H(19D)	107.9
C(19B)-C(20)-H(20A)	91(1)
C(19A)-C(20)-H(20A)	122(1)
C(19B)-C(20)-H(20B)	127(1)
C(19A)-C(20)-H(20B)	106(1)
H(20A)-C(20)-H(20B)	107.4(9)
C(19B)-C(20)-H(20C)	113(1)
C(19A)-C(20)-H(20C)	106(1)
H(20A)-C(20)-H(20C)	106(1)
H(20B)-C(20)-H(20C)	109.4(9)
C(19B)-C(20)-H(20D)	91(1)
C(19A)-C(20)-H(20D)	112(1)
H(20A)-C(20)-H(20D)	30.3(3)
H(20B)-C(20)-H(20D)	129(1)
H(20C)-C(20)-H(20D)	78.1(8)
C(19B)-C(20)-H(20E)	115(1)
C(19A)-C(20)-H(20E)	112(1)
H(20A)-C(20)-H(20E)	78.6(7)
H(20B)-C(20)-H(20E)	32.0(3)
H(20C)-C(20)-H(20E)	132(1)
H(20D)-C(20)-H(20E)	106(1)
C(19B)-C(20)-H(20F)	124(1)
C(19A)-C(20)-H(20F)	102(1)
H(20A)-C(20)-H(20F)	129(1)
H(20B)-C(20)-H(20F)	80.7(8)
H(20C)-C(20)-H(20F)	31.9(3)
H(20D)-C(20)-H(20F)	107(1)
H(20E)-C(20)-H(20F)	109.8(9)
C(22)-C(21A)-O(2)	113(2)
C(22)-C(21A)-H(21A)	109(1)
O(2)-C(21A)-H(21A)	109.0(9)
C(22)-C(21A)-H(21B)	109(1)
O(2)-C(21A)-H(21B)	109.0(9)
H(21A)-C(21A)-H(21B)	107.8
O(2)-C(21B)-C(22)	110(2)

O(2)-C(21B)-H(21C)	110(1)
C(22)-C(21B)-H(21C)	110(1)
O(2)-C(21B)-H(21D)	110(1)
C(22)-C(21B)-H(21D)	110(1)
H(21C)-C(21B)-H(21D)	108.1
C(21A)-C(22)-H(22A)	102(1)
C(21B)-C(22)-H(22A)	120(2)
C(21A)-C(22)-H(22B)	111(1)
C(21B)-C(22)-H(22B)	112(1)
H(22A)-C(22)-H(22B)	112(1)
C(21A)-C(22)-H(22C)	116(1)
C(21B)-C(22)-H(22C)	94(1)
H(22A)-C(22)-H(22C)	109(1)
H(22B)-C(22)-H(22C)	107(1)
C(21A)-C(22)-H(22D)	111(1)
C(21B)-C(22)-H(22D)	112(1)
H(22A)-C(22)-H(22D)	111(1)
H(22B)-C(22)-H(22D)	0.471(6)
H(22C)-C(22)-H(22D)	108(1)
C(21A)-C(22)-H(22E)	116(1)
C(21B)-C(22)-H(22E)	94(1)
H(22A)-C(22)-H(22E)	109(1)
H(22B)-C(22)-H(22E)	107(1)
H(22C)-C(22)-H(22E)	0.729(9)
H(22D)-C(22)-H(22E)	107(1)
C(21A)-C(22)-H(22F)	102(1)
C(21B)-C(22)-H(22F)	120(2)
H(22A)-C(22)-H(22F)	0.599(8)
H(22B)-C(22)-H(22F)	112(1)
H(22C)-C(22)-H(22F)	108(1)
H(22D)-C(22)-H(22F)	112(1)
H(22E)-C(22)-H(22F)	108(1)
Cl(1)#1-C(23)-Cl(1)	112.8(6)
Cl(1)#1-C(23)-H(23A)	109.0(2)
Cl(1)-C(23)-H(23A)	109.0(2)
Cl(1)#1-C(23)-H(23B)	109.0(2)
Cl(1)-C(23)-H(23B)	109.0(2)
H(23A)-C(23)-H(23B)	107.8

Symmetry transformations used to generate equivalent atoms:
#1 -x,y,-z+1/2

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for UltraDemi
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

(6)

	U11	U22	U33	U23	U13	U12
O(1)	63(5)	44(3)	70(4)	23(3)	4(4)	-27(3)
O(2)	84(6)	47(3)	72(4)	-2(3)	48(4)	2(3)
N(1)	63(6)	32(4)	74(6)	10(4)	17(4)	-14(4)
N(2)	42(6)	36(4)	56(5)	6(4)	0(4)	-11(4)
N(3)	41(5)	20(3)	56(5)	1(3)	18(4)	-2(3)
N(4)	44(5)	11(3)	48(4)	2(3)	15(4)	0(3)
C(1)	41(6)	33(5)	42(5)	5(4)	8(4)	-8(4)
C(2)	55(7)	24(4)	41(5)	4(4)	12(5)	-11(5)
C(3)	36(6)	19(4)	45(5)	0(4)	13(4)	-12(4)
C(4)	42(6)	21(4)	28(4)	-1(3)	14(4)	-5(4)
C(5)	39(6)	9(3)	49(5)	-6(3)	19(4)	-7(4)
C(6)	50(7)	12(3)	46(5)	0(3)	21(4)	4(4)
C(7)	38(6)	8(3)	35(4)	0(3)	11(4)	4(4)
C(8)	44(6)	10(3)	37(5)	3(3)	9(4)	4(4)
C(9)	49(6)	14(3)	39(5)	-2(3)	12(4)	-3(4)
C(10)	42(6)	7(3)	36(5)	-6(3)	18(4)	-5(4)
C(11)	36(6)	15(4)	47(5)	3(3)	21(4)	8(3)
C(12)	34(6)	8(3)	52(5)	2(3)	23(4)	3(4)
C(13)	47(6)	14(3)	48(5)	0(3)	20(4)	7(3)
C(14)	55(7)	15(3)	66(6)	0(4)	30(5)	8(4)
C(15)	38(6)	17(3)	58(6)	-1(4)	8(4)	7(4)
C(16)	40(6)	12(3)	38(5)	1(3)	15(4)	1(4)
C(17)	45(6)	21(3)	49(5)	0(4)	12(4)	-6(4)
C(18)	38(6)	31(4)	56(6)	10(4)	7(4)	-4(4)
Cl(1)	102(3)	90(2)	94(2)	-28(2)	40(2)	-43(2)
C(23)	86(13)	33(6)	102(12)	0	-40(10)	0

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for UltraDemi.

	x	y	z	U(eq)
H(5)	2758(2)	16329(8)	6448(6)	38
H(6)	2266(2)	15182(8)	5797(6)	41
H(8)	2622(2)	10232(8)	6579(5)	37
H(9)	3112(2)	11384(8)	7215(6)	41
H(13A)	1840(2)	15000(8)	6003(6)	42
H(13B)	1796(2)	15072(8)	4771(6)	42
H(14A)	1339(2)	16155(8)	5043(6)	51
H(14B)	1312(2)	14496(8)	5759(6)	51
H(15A)	951(1)	14117(6)	4097(4)	47
H(15B)	1228(1)	14309(6)	3546(4)	47
H(16)	1556(1)	10166(6)	4920(4)	35
H(17A)	1080(2)	9638(8)	3658(6)	46
H(17B)	845(2)	11266(8)	3262(6)	46
H(18)	959(2)	9624(9)	5269(6)	51
H(19A)	653(5)	7439(26)	5257(17)	96
H(19B)	766(5)	6819(26)	4273(17)	96
H(19C)	319(7)	8460(31)	5056(19)	96
H(19D)	636(7)	7340(31)	5237(19)	96
H(20A)	100	6625	4320	111
H(20B)	331	5214	4089	111
H(20C)	210	6777	3306	111
H(20D)	81	7050	4001	111
H(20E)	278	5334	4389	111
H(20F)	286	6224	3337	111
H(21A)	498(5)	10967(29)	6096(17)	96
H(21B)	874(5)	11016(29)	6472(17)	96
H(21C)	606(7)	10608(36)	6157(20)	96
H(21D)	324(7)	11821(36)	5492(20)	96
H(22A)	884	13652	6631	139
H(22B)	615	13171	7132	139
H(22C)	535	14153	6055	139
H(22D)	616	13168	7136	139
H(22E)	533	14149	6058	139
H(22F)	883	13660	6626	139
H(23A)	134	565(15)	3046	105
H(23B)	-134	565(15)	1955	105